

An Alternative Transformation for the Elastic and Piezoelectric Constants of Anisotropic Media

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The transformations of the elastic and piezoelectric constants are considered. A new form for these transformations has been derived introducing general Christoffel moduli $\Gamma_t^{(p)}$ ($t = 1 \dots 6$) for the transformation of the elastic stiffnesses and general piezoelectric moduli $E_i^{(p)}$ ($i = 1, 2, 3$) for the transformation of the piezoelectric stress constants, in all cases $p = 1 \dots 6$.

Introduction

The transformation equations for the elastic and piezoelectric constants of anisotropic media referring to a rotated Cartesian coordinate system are well known, being first derived by Voigt (1910). They can also be found in other text books, e.g. Wooster (1938) and Cady (1946). Recently Hearmon (1957) tabulated the equation for the transformation of the elastic and piezoelectric constants of anisotropic media. Various methods of deriving these transformation equations have been used, the most convenient being that of tensor transformation, as the scheme of the elastic stiffnesses form a tensor of the fourth order and that of the piezoelectric stress constants a tensor of the third order in the direction cosines. A very convenient form of equations for transforming the elastic and piezoelectric constants based on tensor application was given by Bechmann in the book 'Piezoelectricity' (1957).

An alternative form of transformation of the elastic and piezoelectric constants has been derived based on the Christoffel elastic moduli and the corresponding piezoelectric moduli. Using the conventional definition of the Christoffel moduli (Christoffel, 1877) which are dependent on the second order of the direction cosines, the transformation for six elastic stiffnesses, e.g., c_{11} , c'_{66} , c'_{55} , c'_{65} , c'_{51} , c'_{16} related to the X' -axis can be obtained as shown by Bechmann (1941). These six Christoffel moduli define the propagation of the three plane waves in an infinitely extended elastic medium. By introducing a more general definition of

the Christoffel moduli, all twenty-one elastic stiffnesses can be defined. Considering, in particular, the propagation of plane waves or of the three thickness modes of infinitely extended plates, this form of transformation is advantageous.

1. Conventional method for transformation of the elastic and piezoelectric constants

The transformed constants are denoted by primes. The twenty-one elastic stiffnesses (elastic moduli) c'_{pq} can be written in general

$$c'_{pq} = \frac{1}{2} \sum_{r=1}^6 \sum_{s=1}^6 c_{rs} (A_{pr} A_{qs} + A_{ps} A_{qr}) \quad (p, q = 1, 2, \dots, 6), \quad (1)$$

where the constants A_{pq} , related to the direction cosines α_{mn} ($m, n = 1, 2, 3$) are shown in Table 1. For $p = q = 1, 2, \dots, 6$, expressions (1) are simplified to

$$c'_{pp} = \sum_{r=1}^6 \sum_{s=1}^6 c_{rs} A_{pr} A_{ps}. \quad (2)$$

Similar expressions hold for the elastic compliances (elastic stiffnesses) s'_{pq} . These expressions differ from those for c'_{pq} by the numerical factors 2 or 4 only. The elastic compliances s'_{pq} are

$$\sigma_{pq} s'_{pq} = \frac{1}{2} \sum_{r=1}^6 \sum_{s=1}^6 \sigma_{rs} s_{rs} (A_{pr} A_{qs} + A_{ps} A_{qr}) \quad (p, q = 1, 2, \dots, 6), \quad (3)$$

where

Table 1

A_{p1}		A_{p2}		A_{p3}		A_{p4}		A_{p5}		A_{p6}	
						A_{p4}^I	A_{p4}^{II}	A_{p5}^I	A_{p5}^{II}	A_{p6}^I	A_{p6}^{II}
A_{11} :	α_{11}^2	A_{12} :	α_{12}^2	A_{13} :	α_{13}^2	A_{14} :	$2\alpha_{12}\alpha_{13}$	A_{15} :	$2\alpha_{13}\alpha_{11}$	A_{16} :	$2\alpha_{11}\alpha_{12}$
A_{21} :	α_{21}^2	A_{22} :	α_{22}^2	A_{23} :	α_{23}^2	A_{24} :	$2\alpha_{22}\alpha_{23}$	A_{25} :	$2\alpha_{23}\alpha_{21}$	A_{26} :	$2\alpha_{21}\alpha_{22}$
A_{31} :	α_{31}^2	A_{32} :	α_{32}^2	A_{33} :	α_{33}^2	A_{34} :	$2\alpha_{32}\alpha_{33}$	A_{35} :	$2\alpha_{33}\alpha_{31}$	A_{36} :	$2\alpha_{31}\alpha_{32}$
A_{41} :	$\alpha_{21}\alpha_{31}$	A_{42} :	$\alpha_{22}\alpha_{32}$	A_{43} :	$\alpha_{23}\alpha_{33}$	A_{44} :	$\alpha_{22}\alpha_{33} + \alpha_{23}\alpha_{32}$	A_{45} :	$\alpha_{23}\alpha_{31} + \alpha_{21}\alpha_{33}$	A_{46} :	$\alpha_{21}\alpha_{32} + \alpha_{22}\alpha_{31}$
A_{51} :	$\alpha_{31}\alpha_{11}$	A_{52} :	$\alpha_{32}\alpha_{12}$	A_{53} :	$\alpha_{33}\alpha_{13}$	A_{54} :	$\alpha_{32}\alpha_{13} + \alpha_{33}\alpha_{12}$	A_{55} :	$\alpha_{33}\alpha_{11} + \alpha_{31}\alpha_{13}$	A_{56} :	$\alpha_{31}\alpha_{12} + \alpha_{32}\alpha_{11}$
A_{61} :	$\alpha_{11}\alpha_{21}$	A_{62} :	$\alpha_{12}\alpha_{22}$	A_{63} :	$\alpha_{13}\alpha_{23}$	A_{64} :	$\alpha_{12}\alpha_{23} + \alpha_{13}\alpha_{22}$	A_{65} :	$\alpha_{13}\alpha_{21} + \alpha_{11}\alpha_{23}$	A_{66} :	$\alpha_{11}\alpha_{22} + \alpha_{12}\alpha_{21}$

$$\sigma_{pq}, \sigma_{rs} = \begin{cases} 1 & \text{for } p, q \text{ or } r, s \text{ equal to } 1, 2 \text{ or } 3 \\ \frac{1}{4} & \text{for } p, q \text{ or } r, s \text{ equal to } 4, 5 \text{ or } 6 \\ \frac{1}{2} & \text{for } p \text{ or } r \text{ equal to } 1, 2 \text{ or } 3 \text{ and } q \text{ or } s \\ & \text{equal to } 4, 5 \text{ or } 6 \text{ (or vice versa).} \end{cases}$$

The transformation equations for the piezoelectric stress constants (piezoelectric moduli) e'_{lq} can be written as

$$e'_{lq} = \sum_{m=1}^3 \sum_{r=1}^6 e_{mr} \alpha_{lm} A_{qr} \quad (l=1, 2, 3; q=1, 2, \dots, 6). \quad (4)$$

This transformation also holds for the piezoelectric stress constants h'_{lq} . The transformations for the piezoelectric strain constants (piezoelectric coefficients) d'_{lq} have a form similar to equation (4) and can be expressed

$$d'_{lq} = \sum_{m=1}^3 \sum_{r=1}^6 \sigma_{mr} d_{mr} \alpha_{lm} A_{qr} \quad (l=1, 2, 3; q=1, 2, \dots, 6), \quad (5)$$

where

$$\sigma_{lq}, \sigma_{mr} = \begin{cases} 1 & \text{for } l, q \text{ or } m, r \text{ equal to } 1, 2 \text{ or } 3 \\ \frac{1}{2} & \text{for } q \text{ or } r \text{ equal to } 4, 5 \text{ or } 6. \end{cases}$$

The piezoelectric strain constants g'_{lq} transform accordingly. Equations (4) and (5) simplify when written in full for the case $l=q=1, 2$ or 3 .

2. An alternative transformation for the elastic and piezoelectric constants

All twenty-one elastic stiffnesses c'_{pq} can be obtained using more generally defined Christoffel moduli. The Christoffel moduli are conventionally defined by Γ_{ik} ($i, k=1, 2, 3$). We introduce Γ_t ($t=1, 2, \dots, 6$) and add the superscript (p) indicating the group of A_{pq} ($p=1, 2, \dots, 6$) as shown in Table 1 in order to form the expressions for the Christoffel moduli. The Christoffel moduli used here are written in the form $\Gamma_t^{(p)}$. For $p=1, 2$ or 3 , the Christoffel moduli are identical

Table 2. The elastic moduli $\Gamma_t^{(p)}$

	A_{p1}	A_{p2}	A_{p3}	A_{p4}^{II}	A_{p4}^{I}	A_{p5}^{II}	A_{p5}^{I}	A_{p6}^{II}	A_{p6}^{I}		
	A_{p1}	A_{p2}	A_{p3}	A_{p4}	A_{p4}^{II}	A_{p5}	A_{p5}^{II}	A_{p6}	A_{p6}^{II}		
	A_{p1}	A_{p2}	A_{p3}	A_{p4}^{I}	A_{p4}^{II}	A_{p5}^{I}	A_{p5}^{II}	A_{p6}^{I}	A_{p6}^{II}		
	$\Gamma_1^{(p)}$	c_{11}	c_{66}	c_{55}	c_{65}	c_{51}	c_{16}	c_{66}	c_{22}		
	$\Gamma_2^{(p)}$	c_{66}	c_{22}	c_{44}	c_{24}	c_{46}	c_{82}	c_{66}	c_{44}		
	$\Gamma_3^{(p)}$	c_{55}	c_{44}	c_{33}	c_{43}	c_{35}	c_{64}	c_{55}	c_{33}		
$\Gamma_4^{(p)\text{II}}$	$\Gamma_4^{(p)}$	$\Gamma_4^{(p)\text{I}}$	c_{65}	c_{24}	c_{43}	$c_{23} \begin{bmatrix} \frac{1}{2}c_{23} \\ + \\ \frac{1}{2}c_{44} \end{bmatrix}$	c_{44}	$c_{45} \begin{bmatrix} \frac{1}{2}c_{45} \\ + \\ \frac{1}{2}c_{63} \end{bmatrix}$	c_{63}	$c_{64} \begin{bmatrix} \frac{1}{2}c_{64} \\ + \\ \frac{1}{2}c_{25} \end{bmatrix}$	c_{25}
$\Gamma_5^{(p)\text{II}}$	$\Gamma_5^{(p)}$	$\Gamma_5^{(p)\text{I}}$	c_{51}	c_{46}	c_{35}	$c_{45} \begin{bmatrix} \frac{1}{2}c_{45} \\ + \\ \frac{1}{2}c_{36} \end{bmatrix}$	c_{36}	$c_{31} \begin{bmatrix} \frac{1}{2}c_{31} \\ + \\ \frac{1}{2}c_{55} \end{bmatrix}$	c_{55}	$c_{56} \begin{bmatrix} \frac{1}{2}c_{56} \\ + \\ \frac{1}{2}c_{41} \end{bmatrix}$	c_{41}
$\Gamma_6^{(p)\text{II}}$	$\Gamma_6^{(p)}$	$\Gamma_6^{(p)\text{I}}$	c_{16}	c_{62}	c_{54}	$c_{64} \begin{bmatrix} \frac{1}{2}c_{64} \\ + \\ \frac{1}{2}c_{52} \end{bmatrix}$	c_{52}	$c_{56} \begin{bmatrix} \frac{1}{2}c_{56} \\ + \\ \frac{1}{2}c_{14} \end{bmatrix}$	c_{14}	$c_{12} \begin{bmatrix} \frac{1}{2}c_{12} \\ + \\ \frac{1}{2}c_{66} \end{bmatrix}$	c_{66}

Table 3. Transformation for the elastic stiffnesses c'_{pq}

	$\Gamma_1^{(1)}$	$\Gamma_2^{(1)}$	$\Gamma_3^{(1)}$	$\Gamma_4^{(1)}$	$\Gamma_5^{(1)}$	$\Gamma_6^{(1)}$	$\Gamma_1^{(2)}$	$\Gamma_2^{(2)}$	$\Gamma_3^{(2)}$	$\Gamma_4^{(2)}$	$\Gamma_5^{(2)}$	$\Gamma_6^{(2)}$	$\Gamma_1^{(3)}$	$\Gamma_2^{(3)}$	$\Gamma_3^{(3)}$	$\Gamma_4^{(3)}$	$\Gamma_5^{(3)}$	$\Gamma_6^{(3)}$	$\Gamma_1^{(4)}$	$\Gamma_2^{(4)}$	$\Gamma_3^{(4)}$	$\Gamma_4^{(4)\text{I}}$	$\Gamma_4^{(4)}$	$\Gamma_4^{(4)\text{II}}$	$\Gamma_5^{(4)\text{I}}$	$\Gamma_5^{(4)}$	$\Gamma_5^{(4)\text{II}}$	$\Gamma_6^{(4)\text{I}}$	$\Gamma_6^{(4)}$	$\Gamma_6^{(4)\text{II}}$									
	$\Gamma_1^{(2)}$	$\Gamma_2^{(2)}$	$\Gamma_3^{(2)}$	$\Gamma_4^{(2)}$	$\Gamma_5^{(2)}$	$\Gamma_6^{(2)}$	$\Gamma_1^{(3)}$	$\Gamma_2^{(3)}$	$\Gamma_3^{(3)}$	$\Gamma_4^{(3)}$	$\Gamma_5^{(3)}$	$\Gamma_6^{(3)}$	$\Gamma_1^{(4)}$	$\Gamma_2^{(4)}$	$\Gamma_3^{(4)}$	$\Gamma_4^{(4)\text{I}}$	$\Gamma_4^{(4)}$	$\Gamma_4^{(4)\text{II}}$	$\Gamma_5^{(4)\text{I}}$	$\Gamma_5^{(4)}$	$\Gamma_5^{(4)\text{II}}$	$\Gamma_6^{(4)\text{I}}$	$\Gamma_6^{(4)}$	$\Gamma_6^{(4)\text{II}}$	$\Gamma_1^{(5)}$	$\Gamma_2^{(5)}$	$\Gamma_3^{(5)}$	$\Gamma_4^{(5)\text{I}}$	$\Gamma_4^{(5)}$	$\Gamma_4^{(5)\text{II}}$	$\Gamma_5^{(5)\text{I}}$	$\Gamma_5^{(5)}$	$\Gamma_5^{(5)\text{II}}$	$\Gamma_6^{(5)\text{I}}$	$\Gamma_6^{(5)}$	$\Gamma_6^{(5)\text{II}}$			
	$\Gamma_1^{(3)}$	$\Gamma_2^{(3)}$	$\Gamma_3^{(3)}$	$\Gamma_4^{(3)}$	$\Gamma_5^{(3)}$	$\Gamma_6^{(3)}$	$\Gamma_1^{(4)}$	$\Gamma_2^{(4)}$	$\Gamma_3^{(4)}$	$\Gamma_4^{(4)\text{I}}$	$\Gamma_4^{(4)}$	$\Gamma_4^{(4)\text{II}}$	$\Gamma_5^{(4)\text{I}}$	$\Gamma_5^{(4)}$	$\Gamma_5^{(4)\text{II}}$	$\Gamma_6^{(4)\text{I}}$	$\Gamma_6^{(4)}$	$\Gamma_6^{(4)\text{II}}$	$\Gamma_1^{(5)}$	$\Gamma_2^{(5)}$	$\Gamma_3^{(5)}$	$\Gamma_4^{(5)\text{I}}$	$\Gamma_4^{(5)}$	$\Gamma_4^{(5)\text{II}}$	$\Gamma_5^{(5)\text{I}}$	$\Gamma_5^{(5)}$	$\Gamma_5^{(5)\text{II}}$	$\Gamma_6^{(5)\text{I}}$	$\Gamma_6^{(5)}$	$\Gamma_6^{(5)\text{II}}$	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$
	$\Gamma_1^{(4)}$	$\Gamma_2^{(4)}$	$\Gamma_3^{(4)}$	$\Gamma_4^{(4)\text{I}}$	$\Gamma_4^{(4)}$	$\Gamma_4^{(4)\text{II}}$	$\Gamma_5^{(4)\text{I}}$	$\Gamma_5^{(4)}$	$\Gamma_5^{(4)\text{II}}$	$\Gamma_6^{(4)\text{I}}$	$\Gamma_6^{(4)}$	$\Gamma_6^{(4)\text{II}}$	$\Gamma_1^{(5)}$	$\Gamma_2^{(5)}$	$\Gamma_3^{(5)}$	$\Gamma_4^{(5)\text{I}}$	$\Gamma_4^{(5)}$	$\Gamma_4^{(5)\text{II}}$	$\Gamma_5^{(5)\text{I}}$	$\Gamma_5^{(5)}$	$\Gamma_5^{(5)\text{II}}$	$\Gamma_6^{(5)\text{I}}$	$\Gamma_6^{(5)}$	$\Gamma_6^{(5)\text{II}}$	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$	$\Gamma_6^{(6)\text{I}}$	$\Gamma_6^{(6)}$	$\Gamma_6^{(6)\text{II}}$			
	$\Gamma_1^{(5)}$	$\Gamma_2^{(5)}$	$\Gamma_3^{(5)}$	$\Gamma_4^{(5)\text{I}}$	$\Gamma_4^{(5)}$	$\Gamma_4^{(5)\text{II}}$	$\Gamma_5^{(5)\text{I}}$	$\Gamma_5^{(5)}$	$\Gamma_5^{(5)\text{II}}$	$\Gamma_6^{(5)\text{I}}$	$\Gamma_6^{(5)}$	$\Gamma_6^{(5)\text{II}}$	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$	$\Gamma_6^{(6)\text{I}}$	$\Gamma_6^{(6)}$	$\Gamma_6^{(6)\text{II}}$	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$	$\Gamma_6^{(6)\text{I}}$	$\Gamma_6^{(6)}$	$\Gamma_6^{(6)\text{II}}$			
	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$	$\Gamma_6^{(6)\text{I}}$	$\Gamma_6^{(6)}$	$\Gamma_6^{(6)\text{II}}$	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$	$\Gamma_6^{(6)\text{I}}$	$\Gamma_6^{(6)}$	$\Gamma_6^{(6)\text{II}}$	$\Gamma_1^{(6)}$	$\Gamma_2^{(6)}$	$\Gamma_3^{(6)}$	$\Gamma_4^{(6)\text{I}}$	$\Gamma_4^{(6)}$	$\Gamma_4^{(6)\text{II}}$	$\Gamma_5^{(6)\text{I}}$	$\Gamma_5^{(6)}$	$\Gamma_5^{(6)\text{II}}$	$\Gamma_6^{(6)\text{I}}$	$\Gamma_6^{(6)}$	$\Gamma_6^{(6)\text{II}}$			
c'_{11}	c'_{66}	c'_{55}	c'_{65}	c'_{51}	c'_{16}	A_{11}	A_{12}	A_{13}	A_{14}	A_{15}	A_{16}	A_{16}	c'_{65}	c'_{24}	c'_{43}	A_{41}	A_{42}	A_{43}	A_{44}	A_{45}	A_{46}	A_{46}	A_{46}	A_{46}	c'_{65}	c'_{24}	c'_{43}	A_{41}	A_{42}	A_{43}	A_{44}	A_{45}	A_{46}	A_{46}	A_{46}	A_{46}			
c'_{66}	c'_{22}	c'_{44}	c'_{24}	c'_{46}	c'_{62}	A_{21}	A_{22}	A_{23}	A_{24}	A_{25}	A_{26}	A_{26}	c'_{66}	c'_{44}	c'_{33}	A_{31}	A_{32}	A_{33}	A_{34}	A_{35}	A_{36}	A_{36}	A_{36}	A_{36}	c'_{66}	c'_{44}	c'_{33}	A_{31}	A_{32}	A_{33}	A_{34}	A_{35}	A_{36}	A_{36}	A_{36}	A_{36}	A_{36}		
c'_{55}	c'_{44}	c'_{33}	c'_{43}	c'_{35}	c'_{54}	A_{31}	A_{32}	A_{33}	A_{34}	A_{35}	A_{36}	A_{36}	c'_{55}	c'_{44}	c'_{33}	A_{41}	A_{42}	A_{43}	A_{44}^{I}	A_{44}^{II}	A_{45}^{I}	A_{45}^{II}	A_{46}^{I}	A_{46}^{II}	c'_{55}	c'_{44}	c'_{33}	A_{41}	A_{42}	A_{43}	A_{44}^{I}	A_{44}^{II}	A_{45}^{I}	A_{45}^{II}	A_{46}^{I}	A_{46}^{II}	A_{46}^{I}	A_{46}^{II}	
c'_{65}	c'_{24}	c'_{43}	c'_{44}	c'_{63}	c'_{25}	A_{41}	A_{42}	A_{43}	A_{44}	A_{45}	A_{46}	A_{46}	c'_{65}	c'_{24}	c'_{43}	A_{41}	A_{42}	A_{43}	A_{44}	A_{45}	A_{46}	A_{46}	A_{46}	A_{46}	c'_{65}	c'_{24}	c'_{43}	A_{41}	A_{42}	A_{43}	A_{44}^{I}	A_{44}^{II}	A_{45}^{I}	A_{45}^{II}	A_{46}^{I}	A_{46}^{II}	A_{46}^{I}	A_{46}^{II}	
c'_{51}	c'_{46}	c'_{35}	c'_{44}	c'_{63}	c'_{25}	A_{41}	A_{42}	A_{43}	A_{44}	A_{45}	A_{46}	A_{46}	c'_{51}	c'_{46}	c'_{35}	A_{51}	A_{52}	A_{53}	A_{54}	A_{55}	A_{56}	A_{56}	A_{56}	A_{56}	c'_{51}	c'_{46}	c'_{35}	A_{51}	A_{52}	A_{53}	A_{54}^{I}	A_{54}^{II}	A_{55}^{I}	A_{55}^{II}	A_{56}^{I}	A_{56}^{II}	A_{56}^{I}	A_{56}^{II}	
c'_{16}	c'_{62}	c'_{54}	c'_{44}	c'_{63}	c'_{25}	A_{51}	A_{52}	A_{53}	A_{54}	A_{55}	A_{56}	A_{56}	c'_{16}	c'_{62}	c'_{54}	A_{51}	A_{52}	A_{53}	A_{54}^{I}	A_{54}^{II}	A_{55}^{I}	A_{55}^{II}	A_{56}^{I}	A_{56}^{II}	c'_{16}	c'_{62}	c'_{54}	A_{51}	A_{52}	A_{53}	A_{54}^{I}	A_{54}^{II}	A_{55}^{I}	A_{55}^{II}	A_{56}^{I}	A_{56}^{II}	A_{56}^{I}	A_{56}^{II}	
c'_{66}	c'_{22}	c'_{44}	c'_{24}	c'_{46}	c'_{62}	A_{61}	A_{62}	A_{63}	A_{64}	A_{65}	A_{66}	A_{66}	c'_{66}	c'_{22}	c'_{44}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	A_{66}^{I}	A_{66}^{II}	c'_{66}	c'_{22}	c'_{44}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	A_{66}^{I}	A_{66}^{II}	A_{66}^{I}	A_{66}^{II}	
c'_{55}	c'_{44}	c'_{33}	c'_{43}	c'_{35}	c'_{54}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	c'_{55}	c'_{44}	c'_{33}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	A_{66}^{I}	A_{66}^{II}	c'_{55}	c'_{44}	c'_{33}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	A_{66}^{I}	A_{66}^{II}	A_{66}^{I}	A_{66}^{II}	
c'_{65}	c'_{24}	c'_{43}	c'_{44}	c'_{63}	c'_{25}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	c'_{65}	c'_{24}	c'_{43}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	A_{66}^{I}	A_{66}^{II}	c'_{65}	c'_{24}	c'_{43}	A_{61}	A_{62}	A_{63}	A_{64}^{I}	A_{64}^{II}	A_{65}^{I}	A_{65}^{II}	A_{66}^{I}	A_{66}^{II}	A_{66}^{I}	A_{66}^{II}	
c'_{51}	c'_{46}	c'_{35}	c'_{44}	c'_{63}																																			

Table 4. The piezoelectric moduli $E_i^{(p)}$

	A_{p1}	A_{p2}	A_{p3}	A_{p4}^{II}	A_{p4}^I	A_{p5}^{II}	A_{p5}^I	A_{p6}^{II}	A_{p6}^I
	A_{p1}	A_{p2}	A_{p3}	A_{p4}	A_{p4}^{II}	A_{p5}	A_{p5}^{II}	A_{p6}	A_{p6}^{II}
	A_{p1}	A_{p2}	A_{p3}	A_{p4}^I	A_{p4}^{II}	A_{p5}^I	A_{p5}^{II}	A_{p6}^I	A_{p6}^{II}
$E_1^{(p)II}$	$E_1^{(p)}$	$E_1^{(p)I}$	e_{11}	e_{25}	e_{36}	e_{31}	e_{15}	e_{16}	e_{21}
$E_2^{(p)II}$	$E_2^{(p)}$	$E_2^{(p)I}$	e_{16}	e_{22}	e_{34}	e_{24}	e_{32}	e_{36}	e_{14}
$E_3^{(p)II}$	$E_3^{(p)}$	$E_3^{(p)I}$	e_{15}	e_{24}	e_{33}	e_{23}	e_{34}	e_{35}	e_{13}

Table 5. Transformation for the piezoelectric stress constants e'_{lq}

	$E_1^{(1)}$	$E_2^{(1)}$	$E_3^{(1)}$	$E_1^{(4)I}$	$E_2^{(4)I}$	$E_3^{(4)I}$	$E_1^{(4)II}$	$E_2^{(4)II}$	$E_3^{(4)II}$
	$E_1^{(2)}$	$E_2^{(2)}$	$E_3^{(2)}$	$E_1^{(5)I}$	$E_2^{(5)I}$	$E_3^{(5)I}$	$E_1^{(5)II}$	$E_2^{(5)II}$	$E_3^{(5)II}$
	$E_1^{(3)}$	$E_2^{(3)}$	$E_3^{(3)}$	$E_1^{(6)I}$	$E_2^{(6)I}$	$E_3^{(6)I}$	$E_1^{(6)II}$	$E_2^{(6)II}$	$E_3^{(6)II}$
e'_{11}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}
e'_{22}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}
e'_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}
e'_{36}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}
e'_{31}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}
e'_{21}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}
e'_{32}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}
e'_{36}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}
e'_{34}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}
e'_{35}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}
e'_{25}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}
e'_{15}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}
e'_{16}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}
e'_{14}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}
e'_{12}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}
e'_{24}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}	α_{11}	α_{12}	α_{13}
e'_{14}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}	α_{21}	α_{22}	α_{23}
e'_{23}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}	α_{31}	α_{32}	α_{33}

with the usual definition. For the following applications, it becomes necessary to split the expressions A_{pq} ($p, q=4, 5, 6$) in Table 1 into two simple products which are denoted as A_{pq}^I, A_{pq}^{II} respectively. The rule of forming the $\Gamma_i^{(p)}$ as indicated in the left-hand column of Table 2 is defined by the subsequent rule of formation: multiply each elastic modulus c_{rs} , as given in the row corresponding to the $\Gamma_i^{(p)}$ of this table, by the corresponding value A_{p1}, A_{p2}, \dots as given at the top of this table, and then add these products. For example, in Table 2, when $p=4$

$$\Gamma_5^{(4)II} = c_{51}A_{41} + c_{46}A_{42} + c_{35}A_{43} + c_{45}A_{44}^{II} + c_{36}A_{44}^I + c_{31}A_{45}^{II} + c_{55}A_{45}^I + c_{56}A_{46}^{II} + c_{41}A_{46}^I.$$

The elastic moduli c'_{pq} as given in the six left-hand columns of Table 3 are obtained by multiplication of the corresponding A_{pq} of each row by the $\Gamma_i^{(p)}$ as given at the top of the table, and then adding these products together. As an example

$$c'_{63} = \sum_{i=1}^3 A_{4i} \Gamma_i^{(5)} + \sum_{i=4}^6 (A_{4i}^I \Gamma_i^{(5)I} + A_{4i}^{II} \Gamma_i^{(5)II}). \quad (6)$$

It can be seen that $c'_{44}, c'_{55}, c'_{66}$ appear three times in this table; $c'_{45}, c'_{46}, c'_{56}$ appear four times; and $c'_{14}, c'_{15}, c'_{16}, c'_{24}, c'_{25}, c'_{26}, c'_{34}, c'_{35}$ and c'_{36} appear twice in this table. This means that these constants can be alternatively expressed. Tables 2 and 3 are self-explanatory. It may be mentioned that the arrangement of the c_{rs} in Table 2 agrees with the arrangement of the c'_{rs} in Table 3.

Similarly, the complete set of 18 piezoelectric stress constants e'_{lq} ($l=1, 2, 3; q=1, \dots, 6$) can be written in terms of generalized piezoelectric moduli $E_i^{(p)}$ ($i=1, 2, 3; p=1, \dots, 6$). These generalized piezoelectric moduli, as indicated in the left-hand column of Table 4, are defined by the rule of formation similar to that of Table 2, but the piezoelectric stress constants e_{lq} are used in place of the elastic stiffnesses c_{pq} . For example, in Table 4 when $p=4$

$$E_2^{(4)I} = e_{16}A_{41} + e_{22}A_{42} + e_{34}A_{43} + e_{24}A_{44}^I + e_{32}A_{44}^{II} + e_{36}A_{45}^I + e_{14}A_{45}^{II} + e_{12}A_{46}^I + e_{26}A_{46}^{II}.$$

The piezoelectric stress constants e'_{lq} as given in the six left-hand columns of Table 5 are obtained by multiplication of the corresponding direction cosines

α_{mn} ($m, n=1, 2, 3$) of the corresponding row of the piezoelectric moduli by the $E_i^{(p)}$ given at the top of the table and then adding these products together. As an example

$$e'_{34} = \sum_{i=1}^3 E_i^{(4)\text{I}} \alpha_{3i}.$$

The piezoelectric stress constants $e'_{14}, e'_{25}, e'_{36}$ appear twice in this table.

A similar form of transformation can be applied to the elastic compliances s'_{pq} and the piezoelectric strain constants d'_{iq} . In Tables 2 and 3, the following substitutions should be made in order to define the elastic compliances:

In place of		Substitute
$\Gamma_i^{(p)}$	$t = 1, 2, \dots, 6$	$\Sigma_i^{(p)}$
c'_{pq} or c_{pq}	$p, q = 1, 2, 3$	s'_{pq} or s_{pq}
c_{pq} or c'_{pq}	$p = 1, 2, 3$ } or vice	$\frac{1}{2}s'_{pq}$ or $\frac{1}{2}s_{pq}$
	$q = 4, 5, 6$ } versa	
c'_{pq} or c_{pq}	$p, q = 4, 5, 6$	$\frac{1}{2}s'_{pq}$ or $\frac{1}{2}s_{pq}$

Correspondingly, Tables 4 and 5 hold for the piezoelectric strain constants when the following substitutions are made:

In place of		Substitute
$E_i^{(p)}$	$p = 1, 2, \dots, 6$	$\Delta_i^{(p)}$
e'_{iq} or e_{iq}	$q = 1, 2, 3$	d'_{iq} or d_{iq}
e_{iq} or e'_{iq}	$q = 4, 5, 6$	$\frac{1}{2}d'_{iq}$ or $\frac{1}{2}d_{iq}$

The piezoelectric strain constants g'_{iq} transform accordingly.

For application to elastic and piezoelectric problems, particularly to thickness vibrations of plates, this transformation is of practical value.

References

- BECHMANN, R. (1941). *Z. Phys.* **117**, 180.
 CADY, W. G. (1946). *Piezoelectricity*. New York; London: McGraw-Hill.
 CHRISTOFFEL, E. B. (1877). *Ann. di Mat. Milano* (II). **8**, 193.
 HEARMON, R. F. S. (1957). *Acta Cryst.* **10**, 121.
Piezoelectricity (1957). British General Post Office, Selected Engineering Reports, London: Her Majesty's Stationery Office (Report No. 1, R. BECHMANN).
 VOIGT, W. (1910). *Lehrbuch der Kristallphysik*. Leipzig: B. G. Teubner.
 WOOSTER, W. A. (1938). *A Text Book on Crystal Physics*. Cambridge: University Press.

Acta Cryst. (1960). **13**, 113

The Electron Density Distribution in Ammonium Bifluoride

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An account is given of a three-dimensional X-ray analysis of NH_4HF_2 based upon Geiger-counter measurements of intensity. The electron density has been measured with a s.d. varying from $0.06 \text{ e.}\text{\AA}^{-3}$ in general positions to $0.11 \text{ e.}\text{\AA}^{-3}$ in special positions. It is found that the electron-density distribution in the H atoms of the NH_4^+ ion corresponds closely to that in an isolated atom with a temperature factor of $\exp(-2.4 \sin^2 \theta/\lambda^2)$. The electron density in the H atoms of the $(\text{FHF})^-$ ions is subject to a rather larger random error, and the results are less clear cut. These atoms have a low peak density (0.47 and $0.52 \text{ e.}\text{\AA}^{-3}$) but the electron count (average) over a sphere of radius 1.1 \AA is normal. There is thus no evidence for a transfer of charge from H to F. The averaged electron density in these two atoms has spherical symmetry, within rather wide limits of error. The F atoms have strongly anisotropic vibrations, and their electron distributions appear to be more diffuse than that in an isolated atom. Attempts to determine the state of ionisation of the N and F atoms were not conclusive. The two independent F-H-F bond distances are 2.275 and 2.269 \AA (s.d. 0.005 \AA), and the N-H distances are both 0.88 \AA (s.d. 0.03 \AA) which is significantly less than the inter-nuclear distance of 1.025 \AA .

Introduction

The fine structure of the bifluoride ion has aroused considerable interest in recent years and has been the

subject of several experimental investigations. Peterson & Levy (1952) give a convenient summary of work done before 1952. It now appears to be established beyond reasonable doubt that the proton is located centrally between the fluorine atoms, and that the original postulate of a double potential well (Ketelaar,

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